

WHAT IS CLAIMED IS:

1. A method for tracking entities in an LC/MS system, comprising:
 - choosing a subset of entities from a first injection
 - choosing a subset of entities from a second injection;
 - comparing the entities chosen from the first injection to those chosen from the second injection;
 - identifying entities chosen from the first injection that match entities chosen from the second injection;
 - constructing a retention time map based on the matching entities;
 - assigning reference retention times based on the retention time map; and
 - tracking entities through the first and second injections using the reference retention times and mass values.
2. The method recited in claim 1, comprising:
 - choosing a coarse retention time threshold;
 - choosing a mass threshold; and
 - choosing the subset of entities from the first injection and the subset of entities from the second injection in accordance with the coarse retention time threshold and the mass threshold.
3. The method recited in claim 1, comprising sorting the matched entities.
4. The method recited in claim 1, further comprising:
 - determining whether an entity has a corresponding entry in the retention time map;
 - using a defined value of retention time if the entity has a corresponding entry in the look-up table;
 - using an interpolated value of retention time if the entity does not have a corresponding entry in the look-up table.
5. The method recited in claim 1, further comprising:
 - determining a fine retention time threshold; and
 - tracking the entities using the fine retention time threshold and mass values.
6. The method recited in claim 1, further comprising:
 - matching entities based on accurate mass and coarse retention time;
 - calculating a delta retention time between matching entities;

filtering the calculated delta retention times;
determining a retention time map using the filtered delta retention times;
determining reference retention times using the retention time map; and
tracking entities through the injections using the reference retention times
and mass values.

7. The method recited in claim 6, wherein the filtering is median filtering.

8. The method recited in claim 1, further comprising filtering the matched
entities.

9. The method recited in claim 8, wherein the filtering is median filtering.

10. A system for tracking entities in an LC/MS system, comprising:

means for choosing a subset of entities from a first injection

means for choosing a subset of entities from a second injection;

means for comparing the entities chosen from the first injection to those
chosen from the second injection;

means for identifying entities chosen from the first injection that match
entities chosen from the second injection;

means for constructing a retention time map based on the matching
entities;

means for assigning reference retention times based on the retention time
map; and

means for tracking entities through the first and second injections using
the retention time map and mass values.

11. The system recited in claim 10, comprising:

means for choosing a coarse retention time threshold;

means for choosing a mass threshold; and

means for choosing the subset of entities from the first injection and the
subset of entities from the second injection in accordance with the coarse
retention time threshold and the mass threshold.

12. The system recited in claim 10, comprising:

means for sorting the matched entities entities.

13. The system recited in claim 10, further comprising:

means for determining whether an entity has a corresponding entry in the
retention time map;

means for using a defined value of retention time if the entity has a corresponding entry in the look-up table;

means for using an interpolated value of retention time if the entity does not have a corresponding entry in the look-up table.

14. The system recited in claim 10, further comprising:

means for determining a fine retention time threshold; and

means for tracking the entities using the fine retention time threshold and mass values.

15. The system recited in claim 10, further comprising:

means for matching entities based on accurate mass and coarse retention time;

means for calculating a delta retention time between matching entities;

means for filtering the calculated delta retention times;

means for determining a retention time map using the filtered delta retention time;

means for using the retention time map to generate reference retention times; and

means for tracking entities through the injections using the reference retention times and mass values.

16. The system recited in claim 15, wherein the filtering is median filtering.

17. The system recited in claim 10, further comprising filtering the matched entities.

18. The system recited in claim 17, wherein the filtering is median filtering.

19. A system for tracking entities in an LC/MS system, comprising:

a liquid chromatograph into which the sample is injected to separate entities in the sample, and to determine a retention time associated with each of the one or more entities;

a mass spectrometer into which the entities are input to determine a mass of each of the one or more entities; and

a computer programmed for:

choosing a subset of entities from a first injection and a subset of entities from a second injection;

comparing the entities chosen from the first and second injections,
identifying matching entities in the first and second injections;
constructing a retention time map based on the matching entities;
assigning reference retention times based on the retention time
map; and

tracking the entities using the retention time map and mass values.

20. The system recited in claim 19, wherein the computer is further programmed
for:

choosing a coarse retention time threshold;

choosing a mass threshold; and

choosing the subset of entities from the first injection and the subset of
entities from the second injection in accordance with the coarse retention time
threshold and the mass threshold.

21. The system recited in claim 19, wherein the computer is further programmed
to sort the matching entities.

22. The system recited in claim 19, wherein the computer is further programmed
for:

determining whether an entity has a corresponding entry in the retention
time map;

using a defined value of retention time if the entity has a corresponding
entry in the look-up table; and

using an interpolated value of retention time if the entity does not have a
corresponding entry in the look-up table.

23. The system recited in claim 19, wherein the computer is further programmed
for:

determining a fine retention time threshold; and

tracking the entities using the fine retention time threshold and mass
values.

24. The system recited in claim 19, wherein the computer is further programmed
for:

matching entities based on accurate mass and coarse retention time;

calculating a delta retention time between matching entities;

filtering the calculated delta retention times;

determining a retention time map using the delta retention times; and

determining reference retention times using the retention time map;
tracking entities through the injections using the reference retention times
and mass values.

25. The system recited in claim 24, wherein the filtering is median filtering.

26. The system recited in claim 19, further comprising filtering the matched
entities.

27. The system recited in claim 26, wherein the filtering is median filtering.